OPTIMAL MESH DESIGN FOR GROUNDWATER FLOW MODELS BASED ON COST AND ERROR CRITERIA

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ABSTRACT

Determining the spatial and temporal discretization is an important part of setting up a model. As a general rule for numerical models, the discretization has to be fine enough on one hand to show most of the details of the solution. At the same time, it cannot be too fine to prevent excessive demand for run time and computer resources.

In this paper, analytical expressions are obtained for optimal mesh size using the physical parameters of the governing ipartial differential equation (PDE), space and time scales under investigation, and run time constraints. The paper describes how sensitive the discretization is to each of the attributes around the optimum.

INTRODUCTION

Unconditionally stable numerical methods using implicit or other methods have made it possible for modelers to use almost any discretization with computer models. Unlike explicit methods where there is some error control because of the stability condition, implicit models such as MODFLOW need guidelines to select discretizations.

Model run time and numerical error are two of the conditions that determine the guidelines. They both depend on the level of discretization. The level of discretization (Δx, Δt) depends on the smallest space and time harmonic that needs to be simulated (k, f) with a given maximum error (ε_T). Out of the three variables (i) $\Delta x, \Delta t$, (ii) k, f, and (iii) ε_T, if two are known, the third can be calculated. The run time, and the storage space are the resources required for model runs. Considering that large model applications need expensive resources, and the chance for making mistakes is high, it is important to understand numerical error and run time before any discretization is finalized.

A number of equations are available to calculate the numerical error in groundwater flow (Lal, 1998, 2000). These expressions use dimensionless spatial and temporal discretizations to describe the error as a percentage of the amplitude of the solution. They provide an upper bound to the numerical error in a given model. Equations are also available for run times of numerical models in terms of the dimensional discretizations. Even if all these equations are derived assuming sinusoidal solutions representing harmonics and assuming boundary disturbances dominate all other stresses, the results

can be useful in model applications in a number of useful ways. Results in the current paper are obtained using these equations.

Design of space and time discretizations in a model application can take place in two stages. In the first stage, the size of the smallest harmonic in space and time that can be observed is determined based on the speed of the available computer and the maximum run time allowed. In the second stage, the discretization needed for obtaining this solution with a specific accuracy is calculated considering that for any harmonic of the solution, a higher accuracy implies a higher level of discretization and a higher cost. Since a model solution consists of many harmonics, once a discretization is selected, it allows harmonics of various other magnitudes to be viewed with various accuracies that can be calculated assuming each harmonic resulted from Fourier's decomposition.

Current study is aimed at understanding the benefits and costs associated with model applications based on numerical error and run time. Expressions are obtained for the optimal discretization based on these criteria.

THEORETICAL BACKGROUND

Two dimensional groundwater flow can be explained using the following governing equation. (Bear, 1979).

$$s_c \frac{\partial H}{\partial t} = \frac{\partial}{\partial x}\left(T_c \frac{\partial H}{\partial x}\right) + \frac{\partial}{\partial y}\left(T_c \frac{\partial H}{\partial y}\right) + \frac{S}{s_c} \tag{1}$$

in which, $H =$ water level or water head; $S =$ summation of source and sink terms representing rainfall, evapotranspiration and infiltration; $T_c =$ aquifer transmissivity; $s_c =$ storage coefficient, all assuming isotropic materials.

Numerical error

Numerical errors are present in computer models because they use discrete values in representing continuous functions explaining flow conditions. Numerical methods can only solve governing equations approximately. For numerical methods based on finite difference methods for groundwater flow equations, an analytical expression can be derived for the numerical error resulting from the truncation of the Taylor series (Hirsch, 1989, Lal, 1998).

$$\varepsilon = 1 - |G| \tag{2}$$

in which, $\varepsilon =$ numerical error per time step as a fraction of the amplitude; $G =$ ratio of amplitudes of numerical and analytical solutions, or the amplification factor of the numerical method.

$$G = \frac{1 - 4d(1-\alpha)\beta \sin^2(\phi/2)}{1 + 4d\alpha\beta \sin^2(\phi/2)} \frac{1}{e^{-d\beta\phi^2}} \tag{3}$$

where $\phi = k\,\Delta x =$ dimensionless discretization in space; $k = 2\pi/\lambda =$ wave number of the harmonic; $\lambda =$ wave length of spatial disturbance; $\psi = f\Delta t =$ dimensionless discretization in time; $f = 2\pi/P =$ frequency; $P =$ period of disturbance; $\beta = \frac{T_c \Delta t}{s_c \Delta x^2} = \frac{\psi}{d\phi^2} =$ mesh ratio; $d = 1, 2$ for one and two dimensional disturbances in square grids. Only 1-D disturbances are looked at in this paper.

The cumulative or maximum numerical error after many time steps, ε_T, depends on the number of time steps n_t, and the error at each time step ε. Error ε_T is bound by $n_t\varepsilon$, in which $n_t = T/\Delta t$.

$$\varepsilon_T \approx \frac{\varepsilon}{\beta\phi^2}\frac{T_c}{s_c}k^2 = \frac{\varepsilon}{d\beta\phi^2}(fT) = \frac{\varepsilon}{\psi}(fT) \tag{4}$$

where, $T =$ maximum duration over which a given harmonic stays in the computational domain and accumulates errors. Considering that harmonics die in the solution domain in diffusion problems, the fate of a disturbance generated at the boundary is useful in calculating a maximum value for T. A value of $(fT) = 1$ is found to be suitable for this approximate calculation (Lal, 2000). Figure 1 shows how the maximum error ε_T calculated using these assumptions show the variation of the error with the level of discretization. Two curves for mesh ratio β of 0.5 and 10 are also shown indicating that $\beta < 0.5$ represents a zone in which an explicit solutions would be viable and $\beta > 10$ represents a zone in which the mesh ratio would be too large. The figure shows that the maximum error rises rapidly as the discretization gets coarser. It is seen that the spatial discretization required is relatively coarser that the temporal discretization because the numerical method is generally second order accurate in space.

Equation (4) can be simplified if ϕ is small by using a truncated Taylor series expansion for ε. For explicit and implicit 1-D and 2-D finite difference schemes,

$$\varepsilon_T \quad \text{(expl/impl 1-D)} \qquad \approx \quad \frac{fT\phi^2}{2}(\mp\beta - \frac{1}{6}) \tag{5}$$

$$\varepsilon_T \quad \text{(expl/impl 2-D)} \qquad \approx \quad fT\phi^2(\pm\beta - \frac{1}{12}) \tag{6}$$

The positive and negative signs apply for the explicit and implicit methods. All these equations for maximum error are valid for problems analyzing boundary stresses. It is assumed for convenience that these equations are also capable of representing errors due to other types of stresses in some form.

Run time

When analyzing the cost of a model run, it is important to consider (1) the capital cost associated with a model setup, which is mainly the cost of a computer system with the required disk space, and (2) the cost of running the model for a given time. The benefit consists of knowing the water levels or the discharges with a certain accuracy. It is not easy to carry out a cost benefit analysis for a model application. However, the following analysis is useful considering that run time is the critical factor in many model applications.

Model run time depends on the speed of the machine and the amount of computations involved. The computer speed (rate of executions) is measured as the number of floating point operations per second c_s (Megaflops) of the computer. The run time for a 2-D finite difference method can be calculated as (Lal, 1998)

$$t_r = \frac{w_u}{c_s}n_t MN = \frac{w_u T_s A f k^2}{c_s \psi\phi^2} = \frac{B}{\psi\phi^2} \tag{7}$$

in which, t_r = run time; $n_t = T_s/\Delta t$ number of time steps; w_u = the number of floating point operations required per cell per time step in the model, to be determined using experimentation for each model; M, N = the number of spatial discretizations in X and Y directions. The number of cells in the domain $= n_c = MN = A/(\Delta x\, \Delta y)$ for rectangular problems in which A = area covered by the model. A variable $B = w_u T_s A f k^2/c_s$ is used to simplify calculations. B represents the number of hours needed for an ideal problem. An easy way to calculate B is to use $B = w_u n_t\, n_c \psi \phi^2/c_s$ from (7) and assume nominal values such as $\phi = 0.5$ and $\psi = 0.2$. Typical values of c_s for the Sun Sparc 20 and a Sun Ultra 2 used for a test are found to be $c_s = 4.1$ and 13.8 Kflops respectively. Dongarra (1998) publishes a list of run times for many other computers. Typical values of w_u are found to be $w_u = 15.7$ and 28.2 Kflops/cell/time step for explicit and successive over relaxation (SOR) models. A value of $w_u = 14.8$ Kflops/cell/time was be obtained for a MODFLOW model using basic, river, drain and well packages with evapotranspiration.

In the case of groundwater problems, the wave number k is related to the disturbing frequency f where $k = \sqrt{f s_c/(2T_c)}$. Now, (7) can be written as

$$t_r = \frac{w_u T_s A f k^2}{c_s \psi \phi^2} = \frac{2 w_u T_s A T_c k^4}{c_s \psi \phi^2} = \frac{w_u T_s A f^2 s_c}{2 c_s T_c \psi \phi^2} \tag{8}$$

which shows that run time can be expressed as a function of f or k. The results show that in a properly discretized model, capturing temporal information half the size is four times more expensive, and capturing spatial information half the size in 1-D is sixteen times more expensive. In the practical design of model applications, (8) is the first equation used to calculate the size of the smallest spatial or temporal feature (k or f) that can be simulated using the model.

The results of this analysis can be used to demonstrate the use of a MODFLOW model with 179 $\times$ 164 square cells of size 150 m and 365 time steps of one day for a simulation. Run time is calculated using (7) as $t_r = 179 \times 164 \times 365 \times 14.8 \times 10^3/(4.1 \times 10^6 \times 3600)$ for a Sparc 10 to give 10.8 Hrs. If $\phi = 0.5$ and $\psi = 0.2$ are assumed, $k = \phi/\Delta x = 0.0033\ m^{-1}$ or the wavelength of the smallest spatial scale simulated is $\lambda = 2\pi/k = 1885$ m. A similar calculation is possible for $f = 0.2\ day^{-1}$ and $P = 31$ days. The value of B can be obtained for this problem using $\phi = 0.5$ and $\psi = 0.2$ in (7) as $B = 0.54$ Hrs. Figure 2 shows the variation of the model run time for this problem focusing on the smallest features mentioned above. The figure shows that run time increases as the discretization gets finer.

Equation (7) for run time, and equation (5) for model error can be combined to obtain a relationship between them. An assumption of small ϕ and a truncation of the higher order terms in (5) is needed for this. The resulting equation is $\varepsilon_T \approx (fT)\, \phi^2 \beta/2 = \psi/2$ for implicit 1-D models when (fT) =1. The relationship between the maximum error and the run time is

$$\varepsilon_T t_r = \frac{w_u T_s A f k^2}{2 c_s \phi^2} = \frac{B}{2\phi^2} \tag{9}$$

Figure 3 shows the variation of the maximum error with the run time for various levels of spatial discretizations. The example shown earlier with $B = 0.54$ Hrs is used for the illustration. For a given spatial discretization identified by a single curve in the plot, variable time steps give an opportunity to traverse through a wide range of ε_T and t_r values. The figure shows that if you start with very small values of ϕ such as 0.1, it is prohibitively expensive to obtain small errors. It also shows that when ϕ is as large as 1.0, the error once again becomes bound. In this example, it is assumed that the model domain described by T_s and A, and the solution harmonic under focus described by f and k remain the same, and only the discretization is varied.

Costs

Consider the following simple expression for the total cost of a model run.

$$C = t_r\, c_r + |\varepsilon_T|\, c_e \tag{10}$$

in which, c_r = cost of running the computer per unit run time in \$/unit time; c_e = the cost associated with increasing the error by 1%. The optimal run time t_{ro} for which the cost is minimum is the point of the tangent of the error versus run time curve and the straight line describing the marginal cost line. At this point,

$$t_{ro} = \sqrt{\frac{B}{2\phi^2}}\sqrt{\frac{c_e}{c_r}} \tag{11}$$

$$\varepsilon_{To} = \sqrt{\frac{B}{2\phi^2}}\sqrt{\frac{c_r}{c_e}} \tag{12}$$

$$\psi_o = \sqrt{\frac{B}{2\phi^2}}\sqrt{\frac{c_r}{c_e}} \tag{13}$$

in which the subscript o represents optimal values. These results show that an optimal time step or ψ_o exists for the problem of linear cost function, and the optimum t_{ro} and ε_{To} values are proportional to the square root of the cost ratio c_e/c_r. If the cost of an error is high and the cost of a run is low, the run time automatically increases.

CONCLUSIONS

Run times and maximum numerical errors are the key factors deciding the discretizations of implicit numerical models for groundwater flow. Very small or very large discretizations may not be suitable for these models because of excessive run time and or numerical error problems. It has been shown that an optimum exists for the size of the discretization once certain cost functions can be assumed. The results show that selecting a discretization is a balancing act. Once selected, a model can be used to see a wide variety of spatial and temporal features with a wide range of accuracies. Large features can be seen with a higher accuracy and small features can be seen with a lower accuracy. The results include actual examples showing the calculation of run time for a MODFLOW model.

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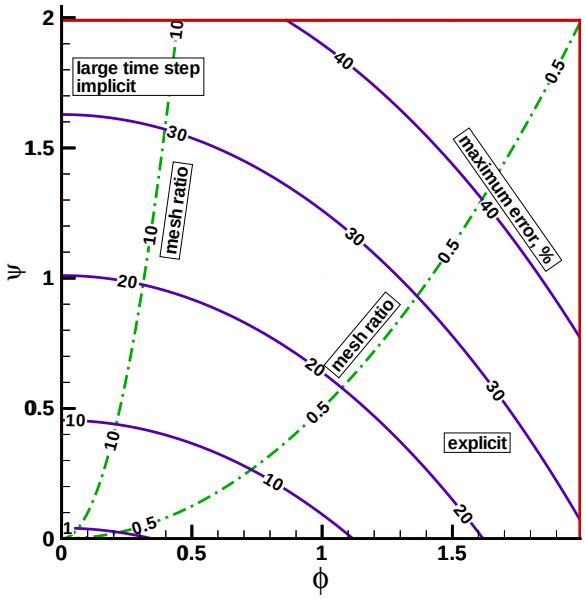

Figure 1: Maximum numerical error as a percentage, as a function of ϕ and ψ.

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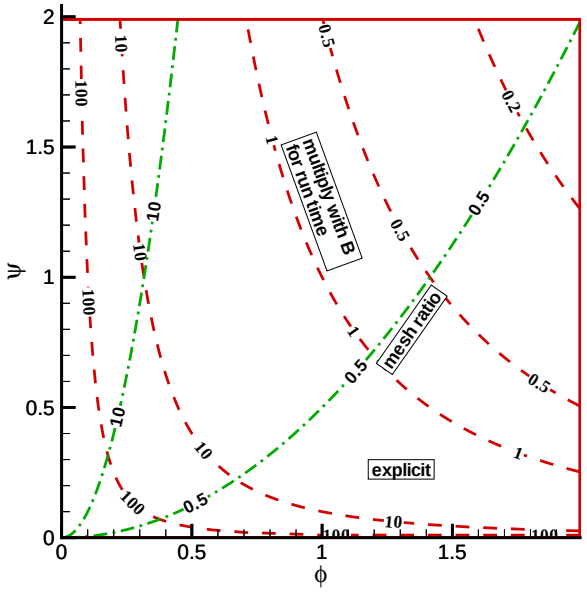

Figure 2: Model run time as a function of ϕ and ψ. To calculate run time, multiply the contour value by B (0.54 Hrs for the example)

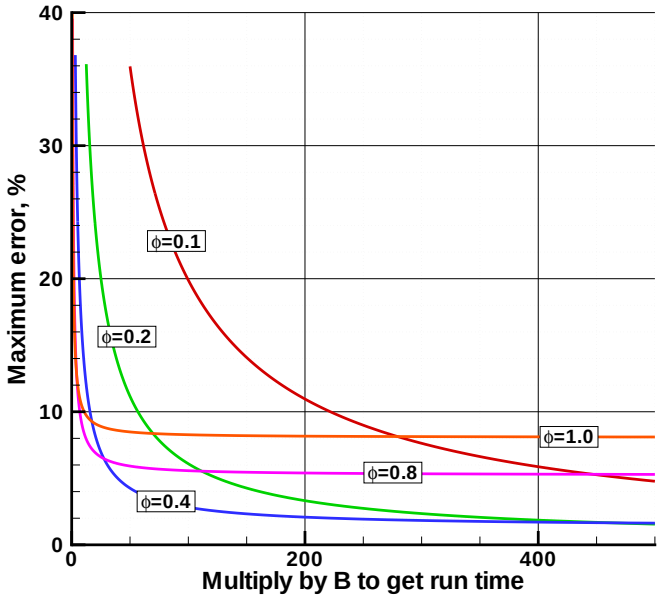

Figure 3: Error versus run time curves for various spatial discretizations ϕ. Multiply the X axis value by B to get the run time